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USING DOMAIN KNOWLEDGE IN EVOLUTIONARY SYSTEM IDENTIFICATION

Marc Schoenauer*

Projet Fractales

INRIA Rocquencourt, B.P. 105

78153 LE CHESNAY Cedex, France

Marc.Schoenauer@inria.fr

<http://www-rocq.inria.fr/fractales/Staff/Schoenauer>

Michèle Sebag

Laboratoire de Mécanique des Solides

Ecole polytechnique

91128 Palaiseau Cedex, France

Michele.Sebag@polytechnique.fr,

<http://www.eeaax.polytechnique.fr/michele>

Abstract. Two example of Evolutionary System Identification are presented to highlight the importance of incorporating Domain Knowledge: the discovery of an analytical indentation law in Structural Mechanics using constrained Genetic Programming, and the identification of the repartition of underground velocities in Seismic Prospection. Critical issues for successful ESI are discussed in the light of these results.

Key words: Evolutionary Optimization, System Identification, Domain knowledge

1 EVOLUTIONARY SYSTEM IDENTIFICATION

In the recent decades, modelisation and simulation of physical phenomena has been widely applied to almost all areas of engineering: from given experimental and initial conditions, the outcome of the physical system are computed, using some (generally simplified) *model* of the underlying phenomena.

Two slightly different situations pertain to System Identification: When the model is totally unknown, the goal is to find the relationship between the input and the output of the whole system, as is the case in the problem presented in section 2. In some other domains, the model itself relies on some sub-model: the *microscopic* behavioral law in Solid Mechanics, the *local* command in control problems, the velocity repartition in the underground (section 3). The goal is then to discover the sub-model that gives correct predictions of the output when used in the higher-level model.

Nevertheless, in both cases, the unknown is a function, and some common issues arise. The most important one is of course the choice of the search space, and some trade-off has to be made: parameterized functional spaces (e.g. spline functions) allow one to use deterministic optimization methods – though the resulting optimization problem generally is highly irregular and multi-modal; on the other hand, unstructured search spaces require stochastic methods – and this explains the

recent progresses in Evolutionary System Identification.

But Evolutionary Computation always faces a dilemma. On the one hand, its flexibility to handle any type of search space opens up huge possibilities, such as searching spaces of graphs, of variable lengths lists, ... Such weird search spaces, being supersets of classical parameterized search spaces, certainly contain better solutions for the problem at hand. On the other hand, the size of these search spaces can hinder the search, and the Evolutionary Algorithm is likely to get stuck in local optima, or to explore only a limited part of the whole search space.

Possible answers to that critical choice is problem specific, and this paper addresses will try to enlighten this issue through two test cases in the area of System Identification Domain knowledge can be used to restrict the search space, as section 2 will demonstrate by introducing a constrained version of Genetic Programming based on Context-Free Grammars in order to cope with dimensional analysis in Structural Mechanics system identification. But even after choosing a smart representation, the search might be hindered by a bad choice of fitness function: section 3 will present an example of identification of the underground in geophysical seismic prospection. In that context, domain knowledge implicitly relies on some common sense assumptions that have to be taken into account explicitly in the Evolutionary Algorithm. General issues related to the introduction of domain knowledge in Evolutionary System Identification will then be discussed in the light of these results in the final section.

2 DIMENSIONAL CONSTRAINTS IN STRUCTURAL MECHANICS

This section focuses on dimensional consistency, a most common background knowledge in scientific domains: given the units associated to the problem variables, the target solution should be a well-formed dimensioned expression (one should not add meters and seconds). All work presented in this section is joint work of the second author with A. Ratle (ISAT, Nevers, France).^{2,3}

2.1 The mechanical problem and dimensionality constraints

The test-case presented here is a simplified real-world application, macro-mechanical modeling from indentation tests. Indentation tests proceed by pressing a hard indenter (of conical or tetrahedral shape) against the surface of the material to be tested out. The experimenter records the reaction force along time and displacement. The target solution (materials behavioral law) expresses force at time t as an analytical function of the materials parameters, and the displacement and its derivative at time t .

The state of the art in Mechanics provides such analytical expressions for simple constitutive laws only For known materials with complex constitutive laws, the indentation law is obtained from computationally heavy simulations (a few hours on an HP350 workstation). For ill-known materials, no indentation law at all is provided. In the two latter cases, behavioral law modeling is a challenge to non parametric model identification.

A standard evolutionary approach to non-parametric identification is Genetic Programming.²⁷ For the sake of procedural simplicity, canonical GP strongly relies on the closure hypothesis (replacing any subtree by another one results in a viable individual). However, the set of dimensionally consistent models is a only tiny fraction of the model set.

Enforcing dimensionality consistency amounts to constraint GP search. One straightforward way to add constraints to any optimization method is to penalize the individuals that violate the constraints. Along this line, a penalisation-based approach has been proposed for dimensionally-aware identification.⁶ However, restricting the search to the feasible space is, when possible, a more efficient approach in Evolutionary Computation.⁷

2.2 Grammar-guided GP

An elegant approach for getting rid of syntactic constraints in GP,⁸ is to combine GP with Backus Naur Form (BNF) grammars. BNF grammars describe the admissible constructs of a language through a 4-tuple $\{S, N, T, P\}$: S denotes the start symbol, N the set of non-terminals, T the set of terminals, and P the production rules. Any expression is built up from the start symbol. Non-terminals are rewritten into one of their derivations as given by the production rules, until the expression contains terminals only.

Interestingly, the construction of any admissible expression through the application of derivation rules, can itself be represented as a tree termed *derivation tree*. *Grammar Guided GP* (G3P) proceeds by exploring the space of derivation trees. The crossover and mutation operators are modified to produce valid derivation trees from valid parents, in the spirit of strongly typed GP.⁹

Generation of Dimensional Grammars

In order to apply Grammar-guided GP to dimensionally consistent identification, a BNF grammar encoding dimensional consistency can be automatically generated, under the restriction that a finite number of units are considered.

In the indentation-based modeling application (section 2.1), the elementary domain units correspond to mass, length and time. Every compound unit is represented by its exponents w.r.t. to the basic units.⁶ Only integer exponents are considered; for instance, the Newton unit ($kg \times m/s^2$) is represented as the triplet $(1, 1, -2)$. In what follows, the exponent of each compound unit is in a given integer range $[-2, 2]$.

To each allowed compound unit (i, j, k) is associated a non terminal $< N_{i,j,k} >$. The associated production rules describes all ways of constructing an expression with type (i, j, k) : by adding or subtracting two expressions of type (i, j, k) ; by multiplying two expressions with types (l, m, n) and (o, p, q) such that $l + o = i$, $m + p = j$, $n + q = k$; and so forth. Finally, the derivation rule associated to the start symbol gives the unit of the target expression (in Newton): $S := < N_{1,1,-2} >$

Initialization

An unexpected difficulty arose during the initialization step. In a non-toy grammar such as above, the fraction of terminal derivations is so small that uniform initialization tends to grow *very* deep and long trees.¹⁰ Adding an upper bound on the depth does not help much: much time is wasted in generating overly long trees, and rejecting them. What is worse, the initial population is ultimately composed of poorly diversified individuals; and final results are poor as evolution hardly recovers from this initial handicap.

A first attempt to solve this difficulty was to select terminals with higher probabilities. Unfortunately, the adjustment of these probabilities proved time-consuming, without significantly improving the diversity in the initial population.

The initialization problem was finally addressed in the spirit of constraint propagation: a depth index is attached to each symbol and derivation in the grammar, and

records the depth of the smallest tree needed to rewrite the symbol into a terminal expression (the index is recursively computed beforehand). From the depth index, one can determine whether a given derivation rule is admissible in order to rewrite a non-terminal symbol in the current expression, i.e. compatible with the total tree depth. Constrained initialization then proceeds by uniformly sampling one among the admissible derivation rules.

2.3 Application

The scalability of G3P has been investigated on the problem of materials behavioral law modeling from indentation tests (section 2.1). Although the grammar size is exponential in the allowed range ($|D| = 5^3 = 125$ non-terminal symbols are considered), its use entails no computational overhead compared to a procedural dimensional consistency check.

One claimed advantage of using background knowledge, e.g. reducing the size of the search space, can be seen by actually computing the sizes of the search spaces for given maximum depths: unconstrained GP gives figures like $8.20125e+5$, $5.54899e+14$ and $3.47438e+23$ for depths of respectively 10, 22 and 34, to be compared to 24, $5.53136e+7$ and $1.02064e+14$ for G3P. Though the size of the search space explored by G3P still grows exponentially with the maximum depth, it demonstrates an exponential gain over GP.

Furthermore, and as could have been expected from statistical learning theory, the reduction of the search space does improve the search efficiency: the results obtained with dimensional grammars always supersede those obtained with untyped grammars by an average of 6 standard deviations.^{2,3}

3 SEISMIC UNDERGROUND PROSPECTION

One of the most challenging problems of the last twenty years in petroleum prospection is the determination of the structure of the underground from data from seismic geophysical experiments. The goal of the inverse problem in seismic reflection is to identify the velocity distribution in the underground from recorded reflection profiles of acoustic waves. All work presented in this section is joint work of the first author with F. Mansanné (Université de Pau et des Pays de l'Adour) in collaboration with the IFP (French Petroleum Institute). All details can be found (in French) in F. Mansanné's PhD, or in other publications^{12,13,14}

3.1 The geophysical problem

A seismic experiment starts with an artificial explosion at some point near the surface. The acoustic waves propagate through the underground medium, eventually being reflected by multiple interfaces between different media. The reflected waves are measured at some points of the surface by some receptors recording the pressure variations along time, called *seismograms*. The identification problem is to identify the repartition of the velocities in the underground domain from the seismograms.

Such geophysical inverse problem results in a highly nonlinear, irregular and multi-modal objective function. Consequently, local optimization approaches, like steepest descent or conjugate gradient, are prone to be trapped in local optima. Hence Evolutionary Algorithms have been long used to tackle this problem.^{15,17,18}

3.2 Representations for underground identification

However, all the above-mentioned works are based on a parametric representation of the underground: either a prescribed layout of the velocities is assumed (the so-called *blocky* model, where velocities are assumed piecewise constant), and the only unknowns are the velocity values themselves;^{15,17} or some global approximation technique is used (e.g. splines¹⁸) and the parameters to identify are the coefficients of that approximation.

Assuming a *blocky* model, and because the fitness computation had to rely on some discretization of the underground domain, one could also think of a parametric representation attaching one velocity value to each element of a given mesh. However, such a representation does not scale up with the mesh size, and/or when going to 3-dimensional problems. Thus, as discussed in¹⁹ in a slightly different context, a non-parametric variable length representation based on **Voronoi Diagrams** was chosen: The genotype is a (variable length) list of points (the Voronoi sites), in which each site is attached a velocity. The corresponding Voronoi diagram is constructed, and each Voronoi cell is given the velocity of the corresponding site.

The variation operators are:¹⁹ a **geometrical** crossover: a random line is drawn across both parents, and the Voronoi sites on one side of that line are exchanged, several mutation operators based on Gaussian mutations of the real-valued parameters, and mutations by addition or destruction of Voronoi sites.

3.3 The fitness functions

The first idea is to use a simulation of the wave equation for the direct problem, and to compare the simulated results to the experimental ones. This standard approach has been used in most previous works.^{15,12} Thus, the identification problem is turned into the minimization of some least square error function (the *LS fitness*).

An alternative approach proposed by the domain experts consists in retrieving the velocity background by using the focusing property of pre-stack depth migration to update the velocity model.^{22,18} In an image gather, each trace represents a migrated image of the subsurface at the same horizontal position. The *Semblance fitness* relies on the fact that reflection events in an image gather are horizontally aligned if the underground velocity model is correct. To measure the horizontal alignment of the reflection events in an image gather, the criterion first proposed in,²³ and applied with success in¹⁷ to 1D seismic profile from the North Sea, has been used.

The main advantage of the migration velocity analysis methods is that they are well understood by geologist experts, and are one order of magnitude faster in terms of computing time compared to solving the wave equation.¹⁵

3.4 Results

Due to its lower computational cost, and because the domain experts considered it a more robust criterion than the least square comparison of simulated and experimental seismograms, first experiments on realistic models of the underground (the IFP model *Picocol*) used the the Semblance fitness ... with disastrous results:¹³ the experimental seismograms were actually simulated on known synthetic models of the underground, so the solution was known. However, some totally unrealistic solutions emerged, that had better Semblance than the actual solution. Of course, such parasite solutions would never have been retained by even first grade students in Geophysics. But there was nowhere in the modelisation of the problem where such

common sense argument could be added (e.g. sandwiches of low velocity between two layers of very high velocity).

On the other hand, using the LS fitness based on a numerical simulation of the wave equation did not exhibit this defect on coarse discretization,¹² but proved far too costly for more realistic discretizations. A compromise was finally set up and successfully used: alternating both methods, i.e. using the Semblance fitness during a few (5-10) generations, then the LS fitness during some (2-5) generations, proved both robust (weird solutions with good Semblance were eliminated by the few generations using LS fitness) and not too costly (in addition, an increasing number of shots were taken into account - one wave equation must be solved for each shot).

The best results for some subset of the Picrocol model discretized according to a 80×70 mesh reached an average relative error of around 12%, less than 5% in 3/4 of the domain, but still required 200h of Silicon O2 computer for 20000 evaluations of each fitness. These results were considered very encouraging by the domain experts.

4 Discussion and conclusion

The choice of a representation very often is dictated by ... the target optimization method. Indeed, the only optimization methods that have been around for a long time in the Applied Maths field are the standard deterministic numerical optimization methods that are only defined on *parametric search spaces* (i.e. looking for vectors of real-numbers). Hence, the first thought of a numerical engineer facing an optimization problem is to transform that problem into a parametric optimization problem. However, such transformation might imply some restrictions on the search space, making optimal solutions of the original problem out of reach. A good example is given on the geophysical test-case (section 3.2) where splines, or fixed-complexity blocky models had been used exclusively because the resulting problem amounted to parametric optimization. It is interesting to note that even the first Evolutionary approaches did not question the representation

On the opposite, choosing a very general representation that adds the least possible limitations on the problem might result in a huge search space, where indeed some very good solutions lie, by in which the exploration might be very difficult, resulting in sub-optimal solutions too. It is then necessary to restrict the search to some particular regions of the search space. However, there are generally many regions of those huge general search space that common sense considerations could easily prune – but EAs lack common sense!

On the seismic prospection problem (section 3.2), the search space should be further reduced: for instance, experts very well know that there are not large jumps of velocity values between the different blocks, that deep parts of the underground cannot have small velocities, etc But such considerations are very difficult to take into account. On the opposite, in the Mechanical problem of section 2, expert knowledge (dimensional analysis) is the basis of the restriction of the huge GP search space.

Dual to the choice of a representation is the choice of variation operators (mutation, crossover and the like). It has been argued that a proper choice of representation could naturally lead to good operators²⁴ – and indeed such approach certainly avoids using useless (i.e. meaningless for the problem at hand) operators. However, domain knowledge can also clearly help improving such representation-independent operators. For instance, the crossover operator based on simple geometrical consid-

erations used for the Voronoi representation described in section 3.2 does outperform the blind exchange of Voronoi sites.²⁵

Similarly, the initialization is another part of an Evolutionary Algorithm where domain knowledge can usefully step in. Initialization is very often taken for granted in Evolutionary Algorithms, e.g. a common advice is to perform a uniform sampling of the search space.

First, even when such a uniform distribution does exist on the search space, some problem specific issues might lead to non-uniform initialization.²⁶ But there are many cases where nothing like a uniform distributions on the search space actually exists. Hence some *ad hoc* procedures have to be designed, and domain knowledge is mandatory there, too. A very simple example is the case of unbounded real parameters, where some distribution has to be arbitrarily chosen (e.g Gaussian with given standard deviation, uniform on a bounded interval, ...). This is of course even more difficult in the case of variable length representations. In standard GP, for instance, the now-standard ramp half-and-half procedure²⁷ took some years to design. Finally, restricting the search space as is done in the Structural Mechanics example also implies modifying the initialization procedure, and that might prove quite difficult (see section 2.2).

Last but not least, the choice of the fitness function must be addressed with care – and this might be surprising to many researchers: the objective function is generally the starting point and is very often never even discussed. But that starting point very often is already the result of some simplification, or some choice from the modeling engineer – and he might have made the wrong choice on some important decision. For instance, though the least square comparison is generally preferred, the maximum difference is another possibility in the simple case where the objective function is built on the aggregation of different fitness cases. Moreover, as demonstrated in section 3, some widely accepted objective functions might in fact assume some common sense rules that do not exist – and will be very difficult to add – in the Evolutionary Algorithm that will actually solve the problem.

In summary, we believe that Evolutionary Algorithms will have a large impact in System Identification – similarly to that of Artificial Creativity in the area of Design.²⁹ However, there are many obstacles on the road to success, and this paper has tried to highlight some of them, hoping that this will make future evolutionary engineers ask themselves the important questions before entering the optimization loop.

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